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Algorithmic Issues for Scaling Structured AMR Calculations to Thousands of Processors

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with

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Center for Applied Scientific Computing

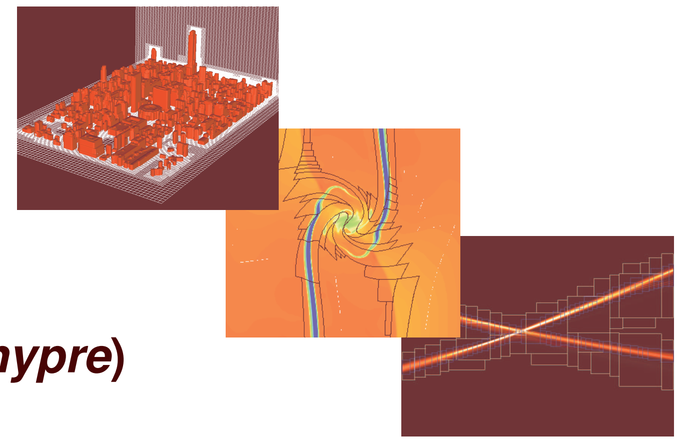
Outline

- Structured Adaptive Mesh Refinement (SAMR) overview
- Parallel implementation approaches used in SAMRAI
- Scaling issues on O(1000) processors
- Predictions of scaling issues on O(100,000) processors

SAMRAI

Structured Adaptive Mesh Refinement Application Infrastructure

- **SAMRAI provides parallel AMR support to applications**
  - **High-level reusable AMR algorithms (e.g. timestepping, dynamic grid generation)**
  - **Parallel support (MPI)**
  - **Parallel tools (VAMPIR, TAU)**
  - **Checkpointing & restart support (HDF)**
  - **Interfaces to solvers (PETSc, PVODE, *hypre*)**



Current SAMRAI users regularly run on large processor systems

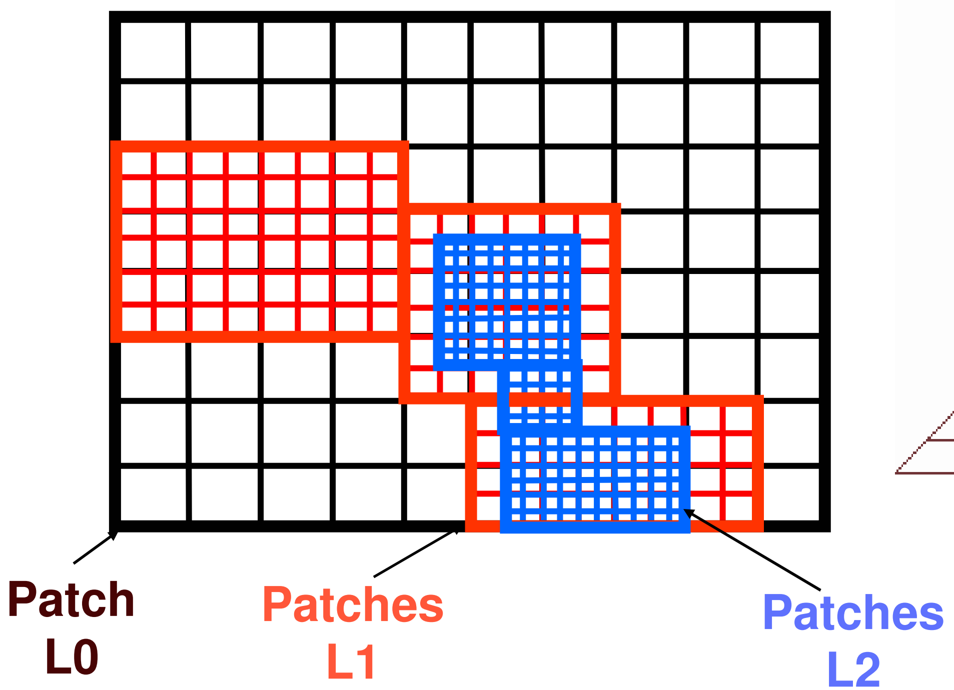
MCR Linux cluster

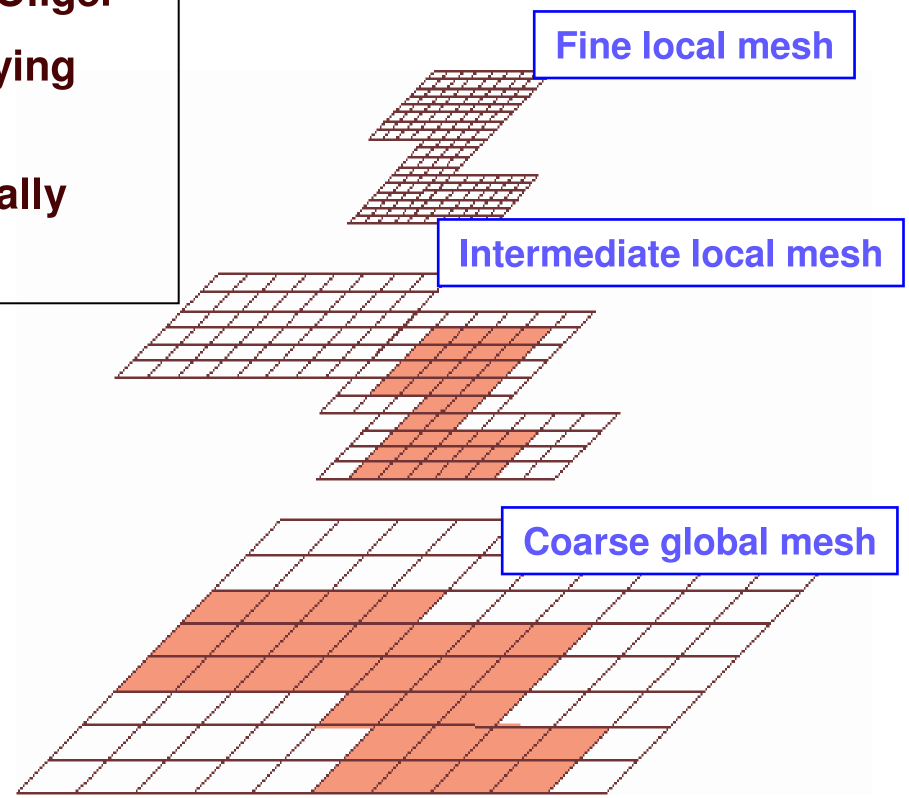
IBM Blue Pacific

TC2K Alpha cluster

Structured AMR (SAMR) employs a dynamically adaptive "patch" hierarchy

- Based on methods of Berger, Colella, Oliger
- Hierarchy defines nested levels of varying mesh resolution
- Data stored on patches covering logically rectangular index space



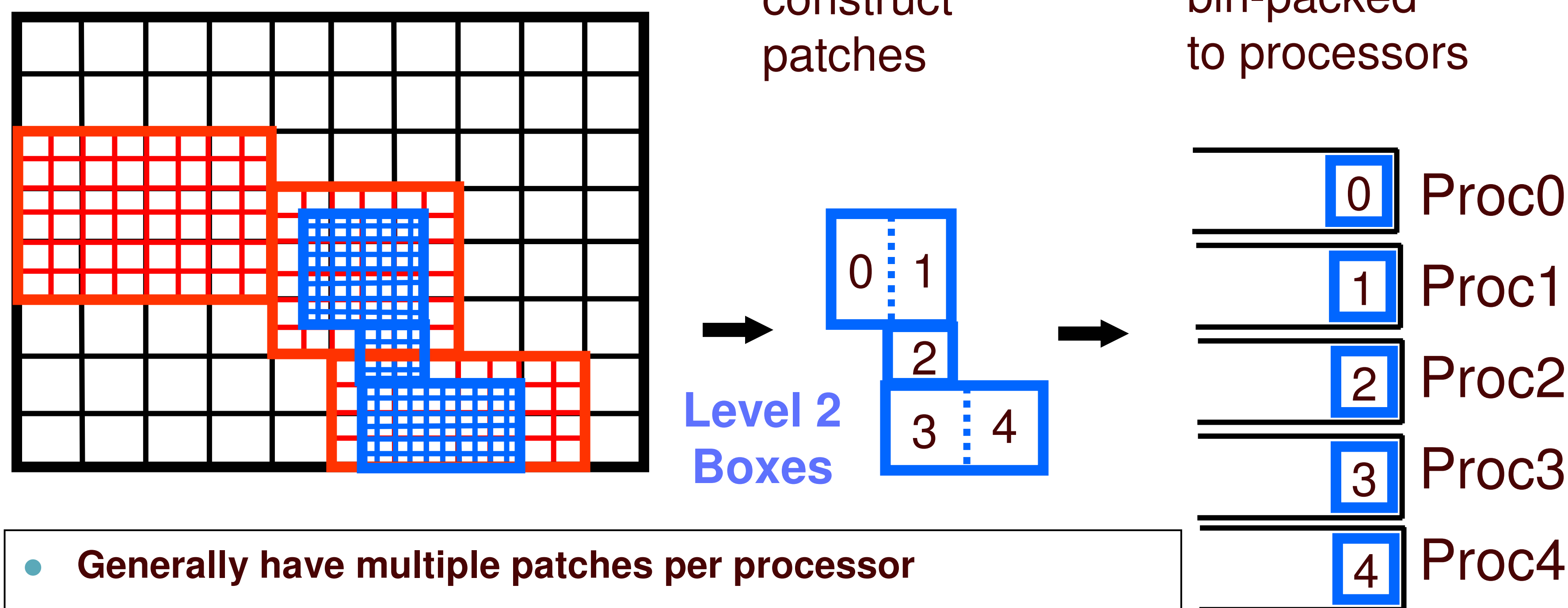


Patches distributed to processors to balance computational workload

1) Box regions constructed

2) Boxes split to construct patches

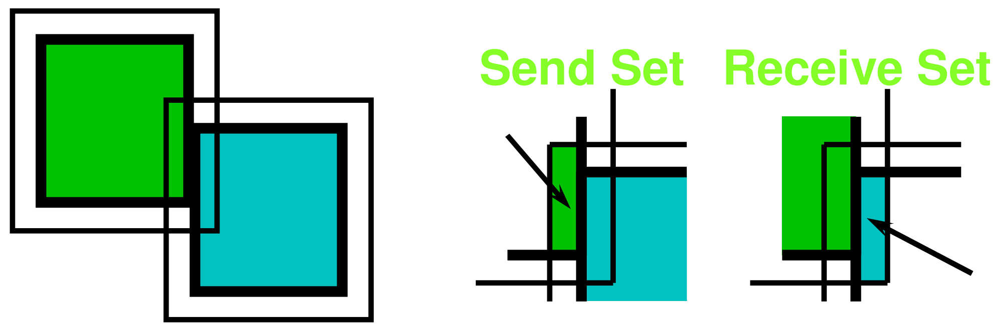
3) Patches bin-packed to processors



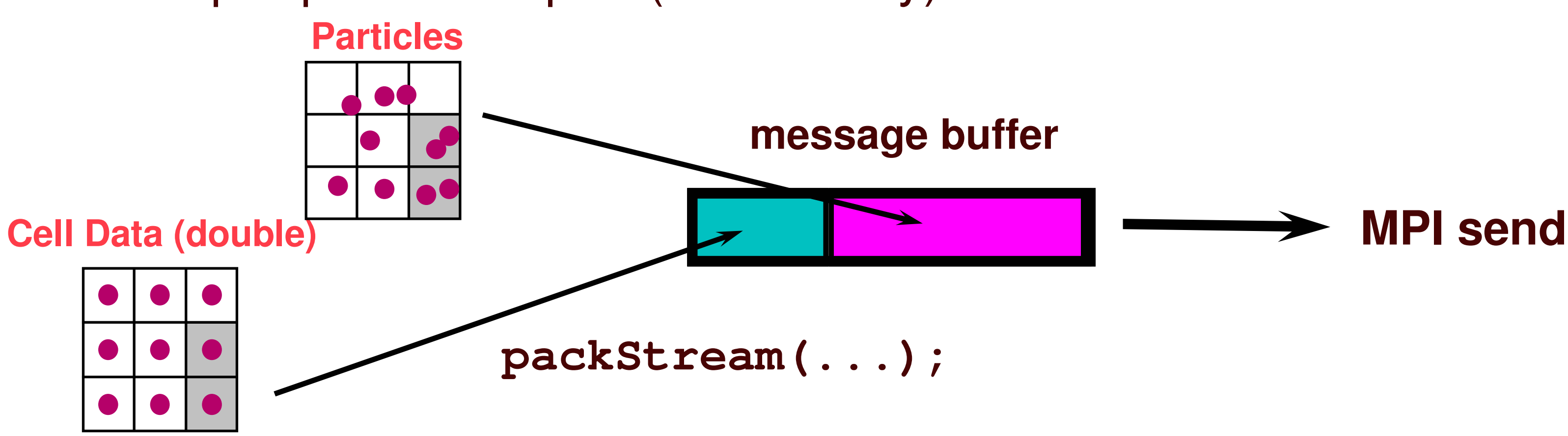
- **Generally have multiple patches per processor**
- **Each level load balanced separately**
- **Spatial bin packing may be used to maintain locality of patches on processors**

Communication schedules create and store data dependencies

- **Amortize cost of creating send/receive sets over multiple communication cycles**

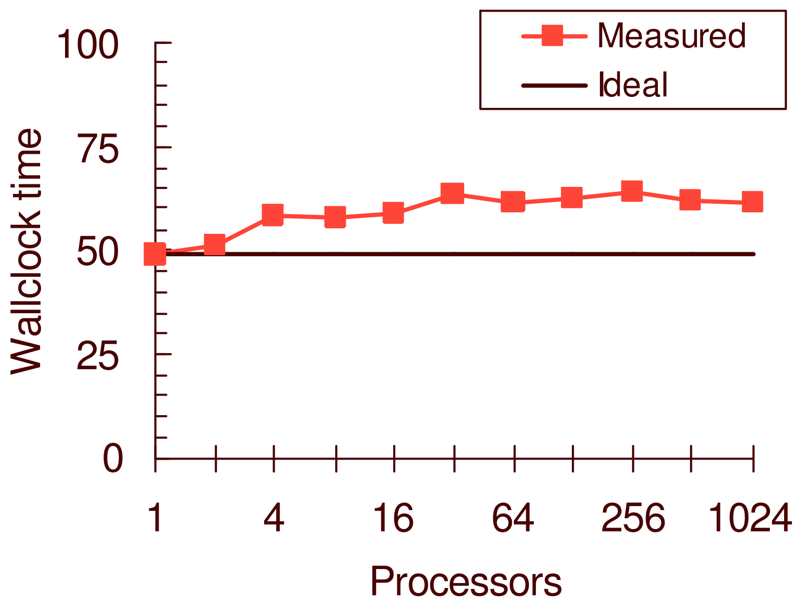


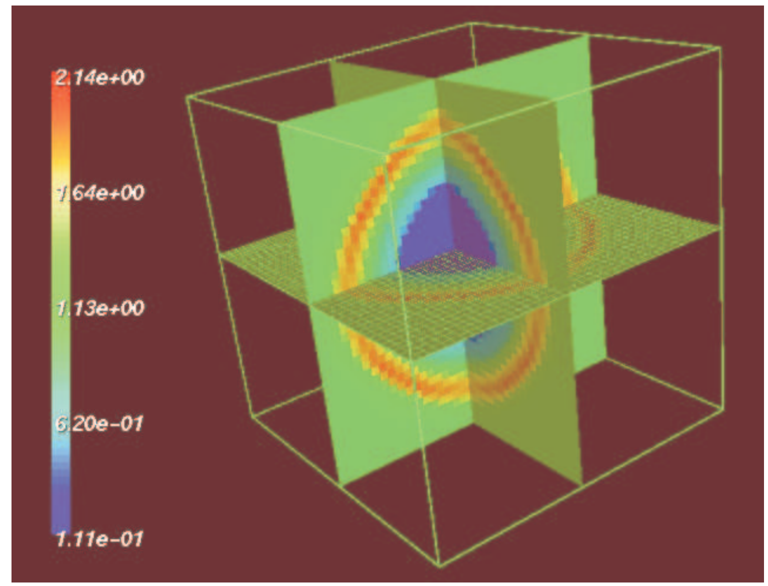
- **Data from various sources packed into single message stream**
  - supports complicated variable-length data
  - one send per processor pair (low latency)



Non-adaptive calculations using SAMRAI show good scaling

Scaled speedup for non-AMR hydro calculation





- Majority of computational spent in patch integration routines. Library code < 5% of total wallclock time

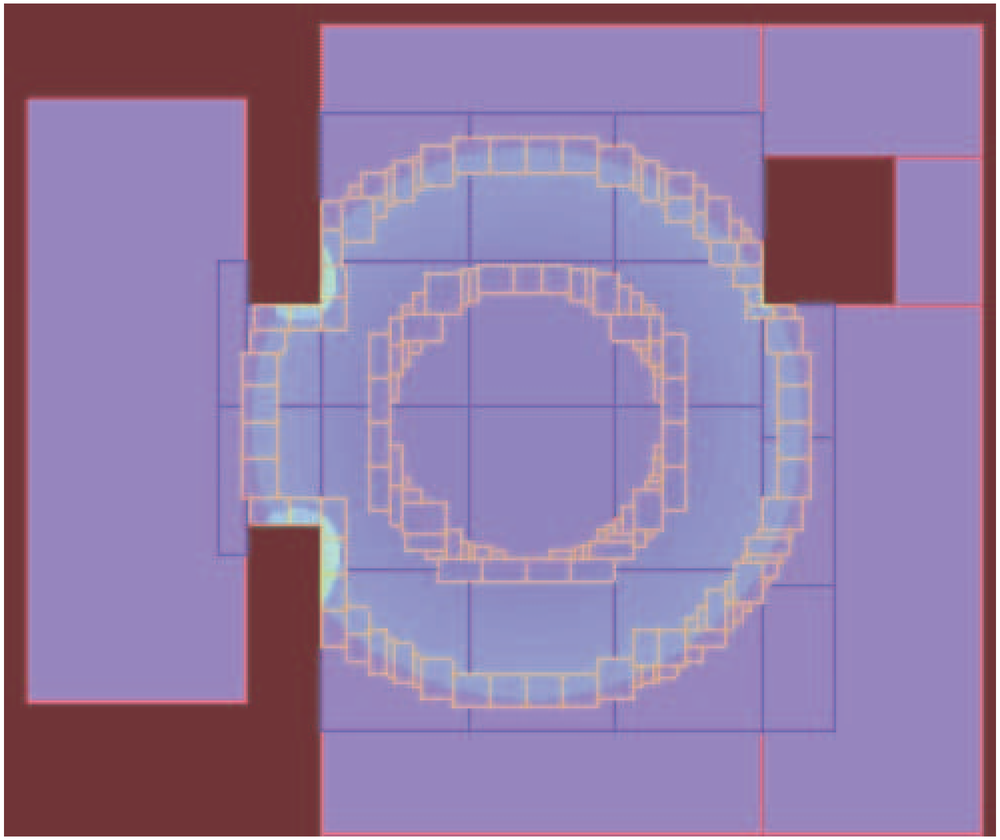
Dynamic mesh adapts to features as solution evolves

Adaptive solution of Euler equations

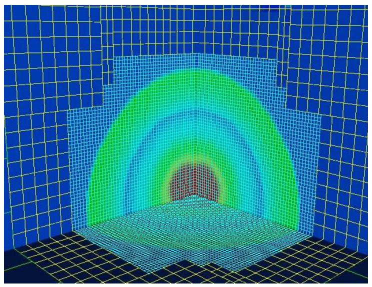
Initial conditions:

inside sphere
density = 8.0
pressure = 40.0

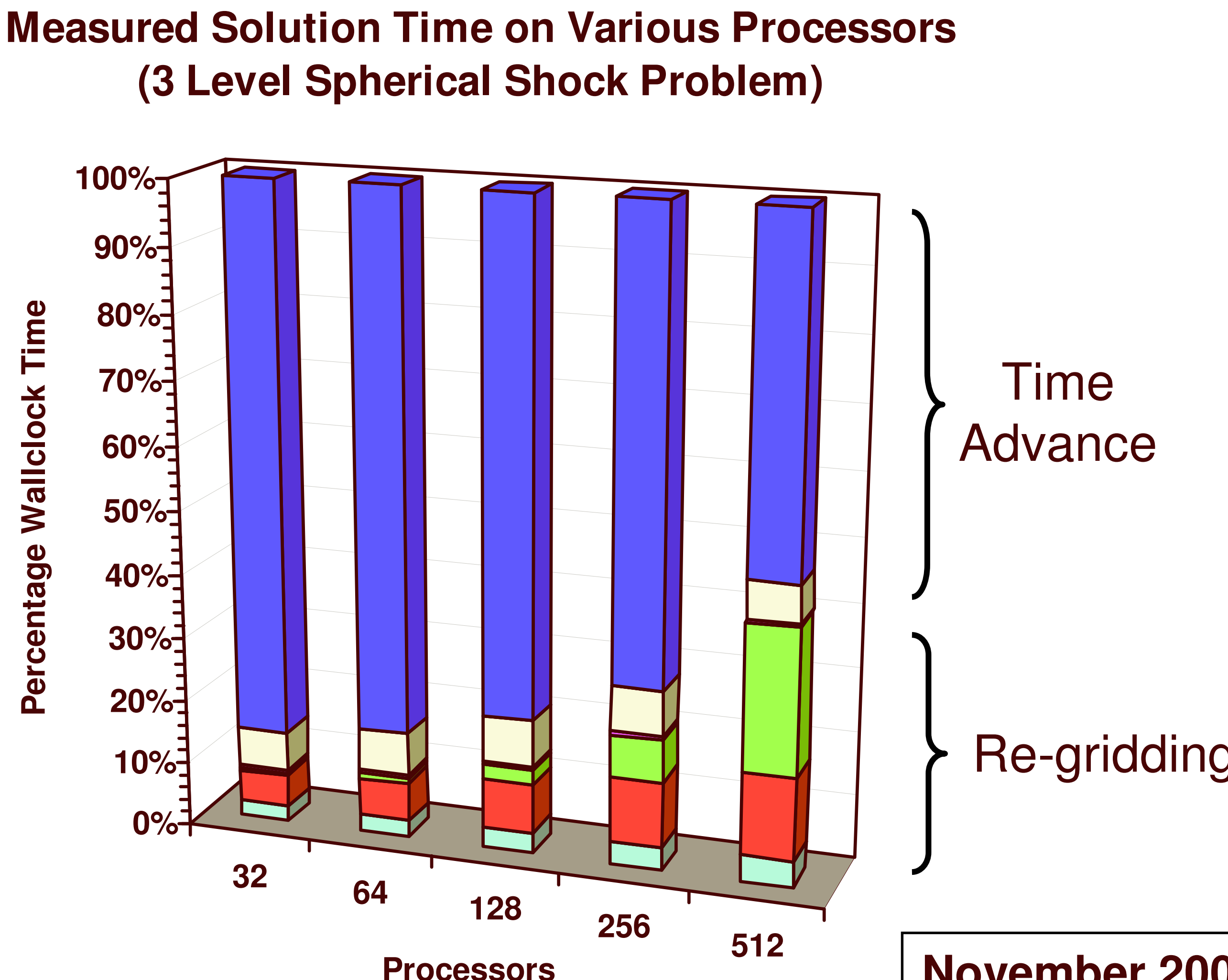
outside sphere
density = 1.0
pressure = 1.0



Adaptive problems show poor scaling in dynamic gridding operations



Non-scaled Euler calculation
IBM Blue Pacific

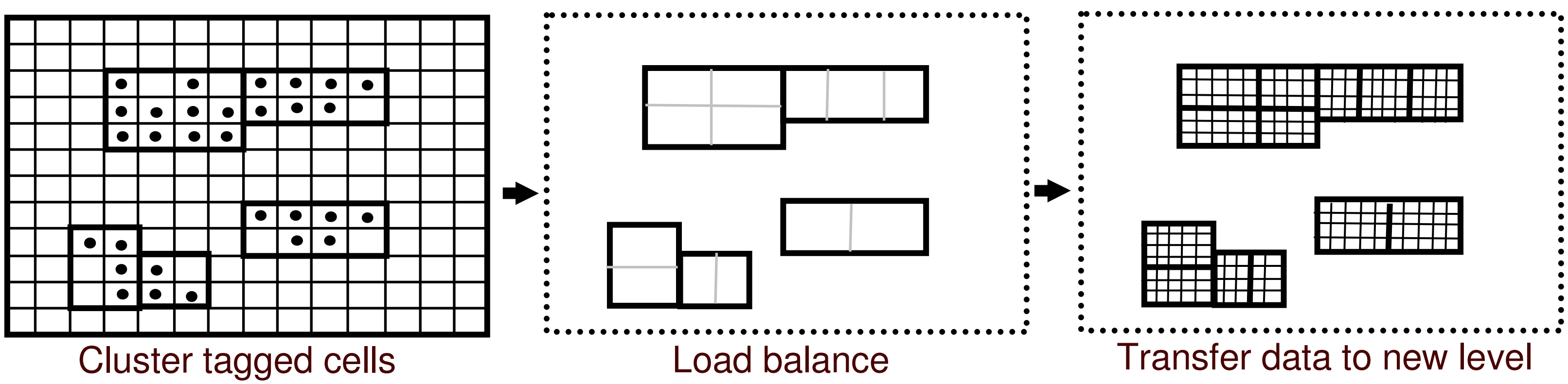


November 2001

Summary of what we mean by “adaptive gridding”

Steps required to construct a new refinement level:

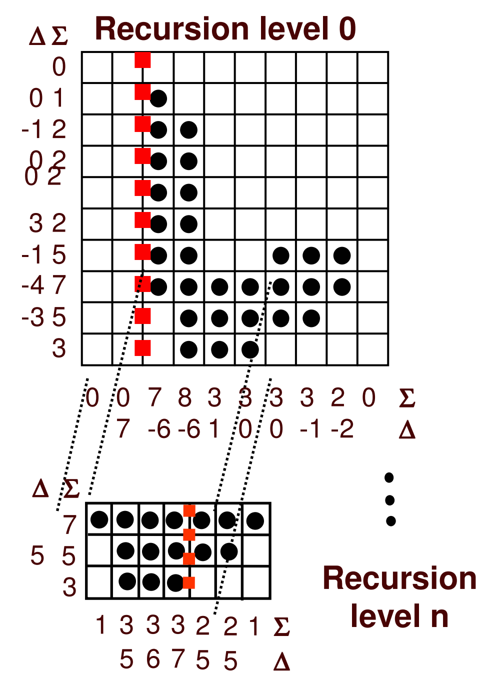
		% Total Time
1.	Tag cells (on coarser level) requiring refinement	< 1%
2.	Cluster tagged cells into “box” regions	1% - 46%
3.	Cut up “box” regions into smaller boxes and determine processor distribution (I.e. load balance)	< 1%
4.	Recompute communication schedules	2% - 87%
5.	Transfer data from old to new level	1-2%



Tagged Cell Clustering Algorithm (Berger Rigoutsos)

- **Original implementation utilized global reductions to construct box histograms**
  - Scales poorly with problem size – number of global reductions grows by $O(n^2)$ (n = number gridcells)
  - Scales poorly with processor count – cost of each global reduction is O(PlogP) (P = number processors)

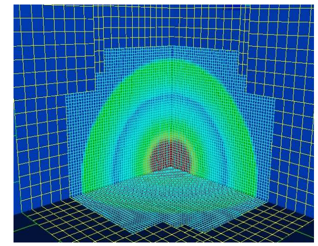
- **Replaced with a new “manager/worker” implementation**
  - Only processors holding tags participated in communication
  - Manager processor accumulates tag histograms and distributes resulting boxes to all processors



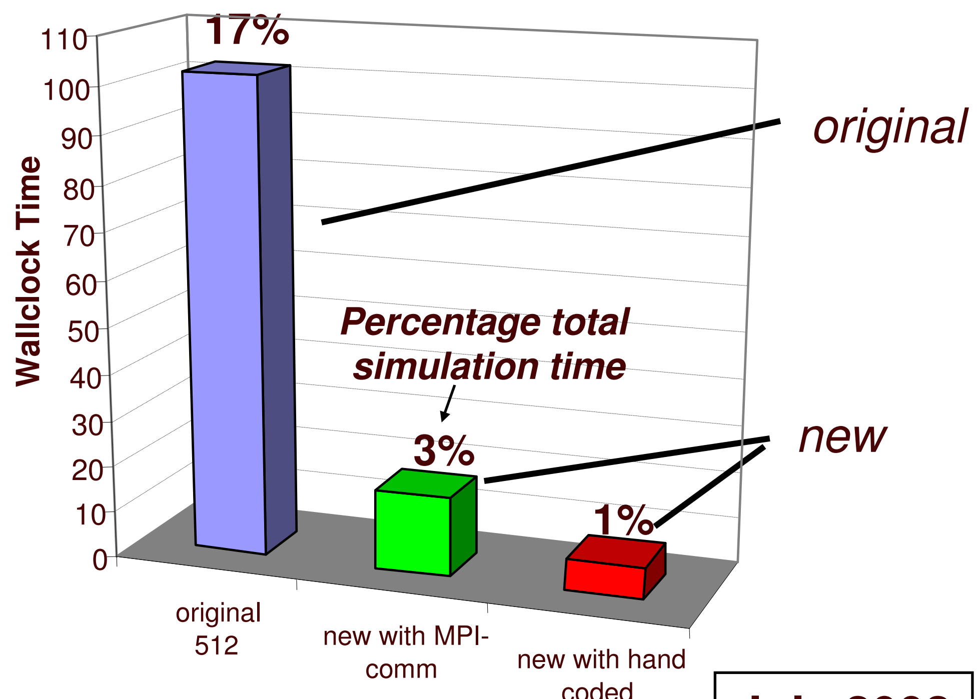
New implementation significantly reduces clustering costs

- **Hand coded MPI send/recvs more effective than MPI communicators**
- **Most significant improvement on systems with slow global reductions**
  - Blue pacific has slower global reductions than newer IBM systems
  - Less significant improvement observed on Linux MCR system

Non-Scaled Euler calculation
IBM Blue Pacific



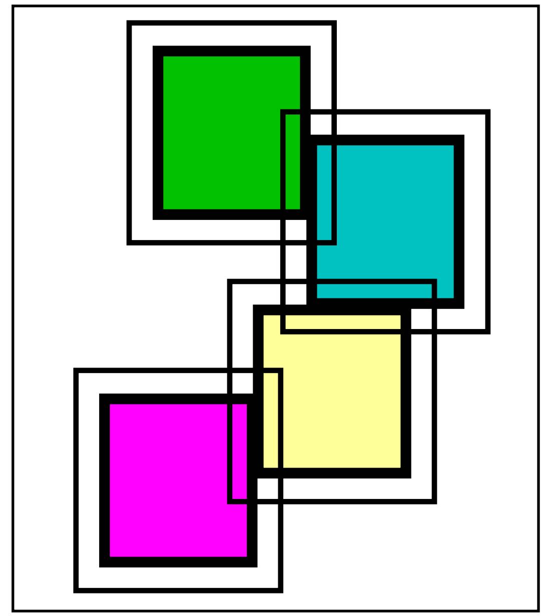
Berger-Rigoutsos – 512 processors



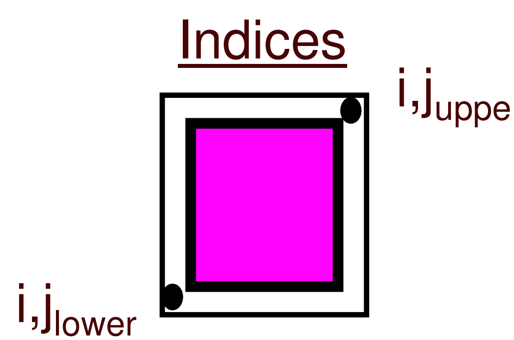
July 2002

Complexity in Comm. Sched. construction becomes significant in large problems

- Data dependencies between patches determined by identifying intersections.
- Original algorithm compared each patch index with all others in the problem.
- Complexity $O(N^2)$ N = number of patches

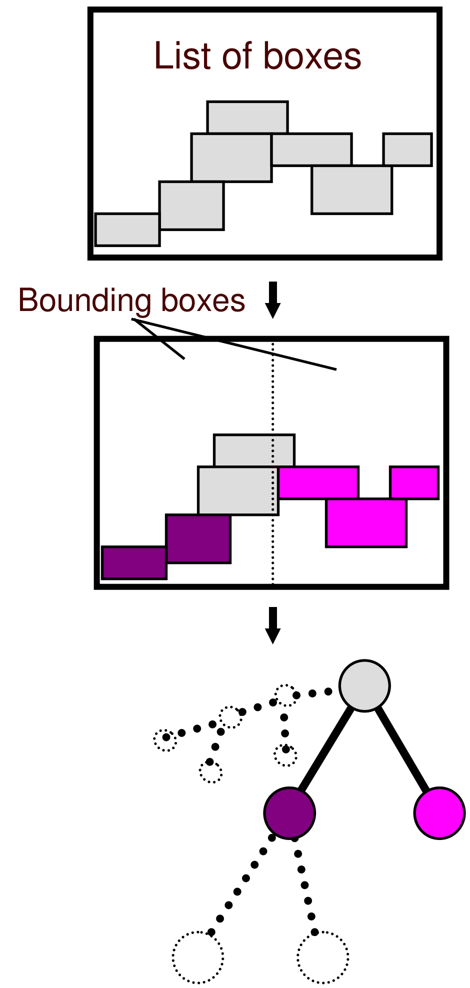


→ ***Communication schedule construction costs grow $O(N^2)$ with problem size***

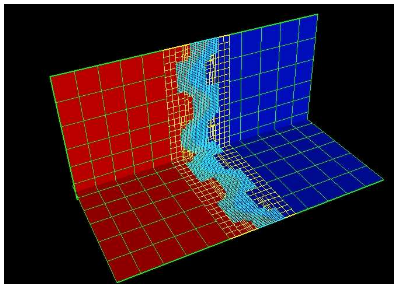


Recursive Binary Box Tree (RBBT) efficiently describes spatial relationships

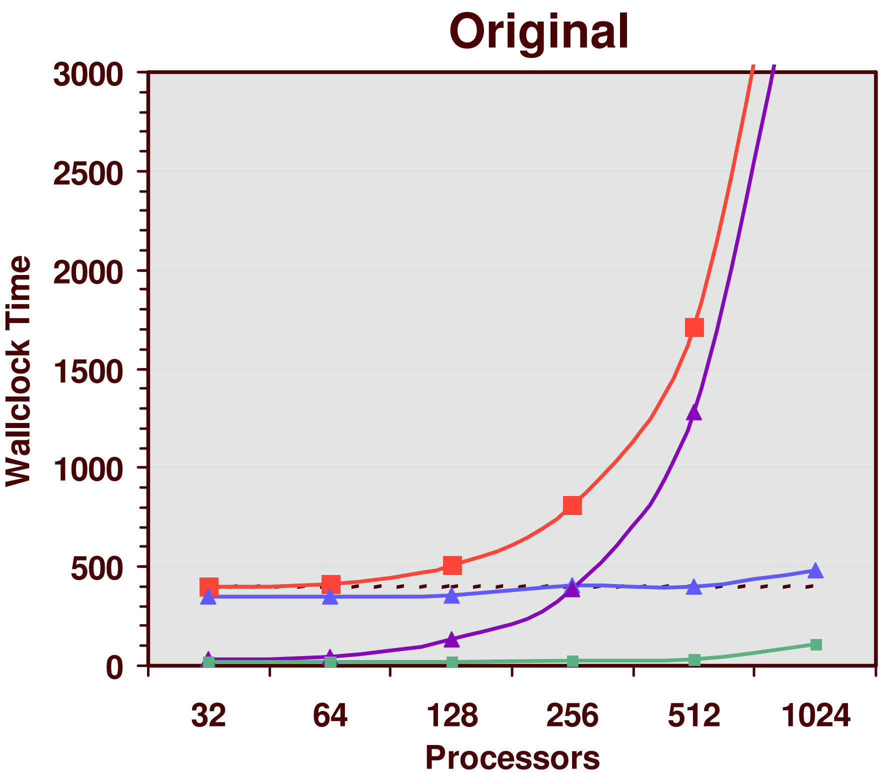
- **Fast determination of box intersection**
- **Analogous to Octree representation**
  - uses bounding boxes and boxlists rather than cells and sub-cells
  - For any given box, determines small subset of boxes that will possibly intersect it, for which we can apply naïve $O(N^2)$ algorithm.
- **Complexity analysis:**
  - Setup: O(N log(N))
  - Query: walk the trees: O(log(N)) per box
  - Runtime complexity: O(N log(N)) – approximate, may vary for different box layouts.

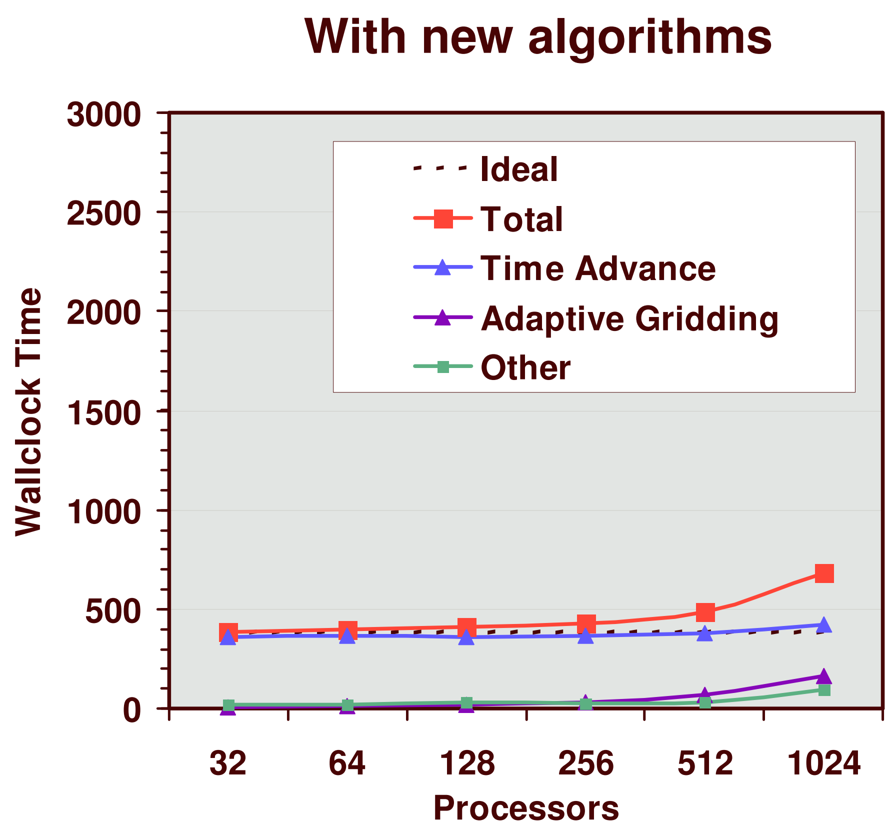


Parallel performance of scaled linear advection benchmark

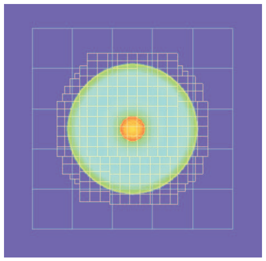


Scaled
3 level linear advection problem
Linux MCR Cluster

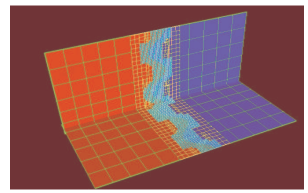




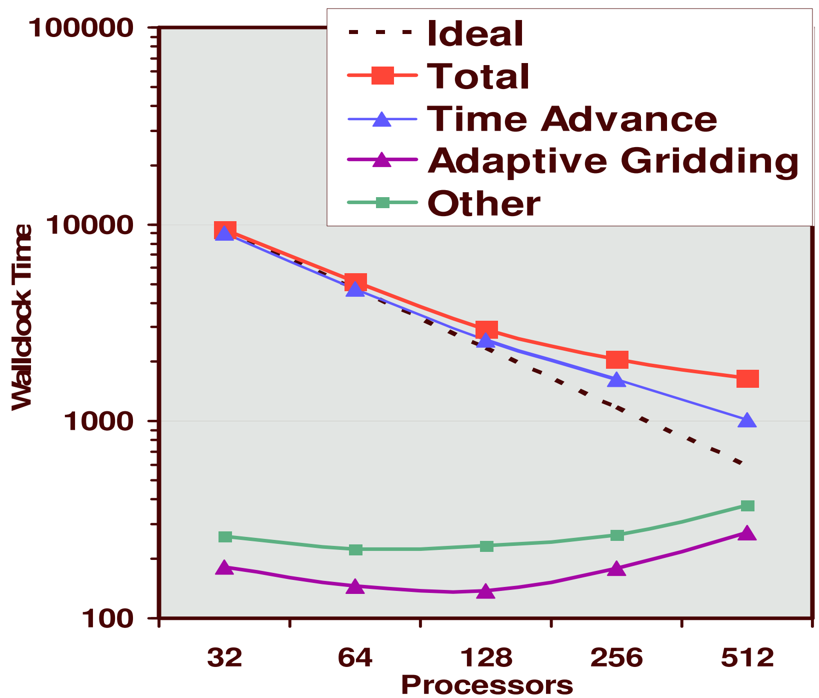
Scaling results after adaptive gridding algorithm modifications

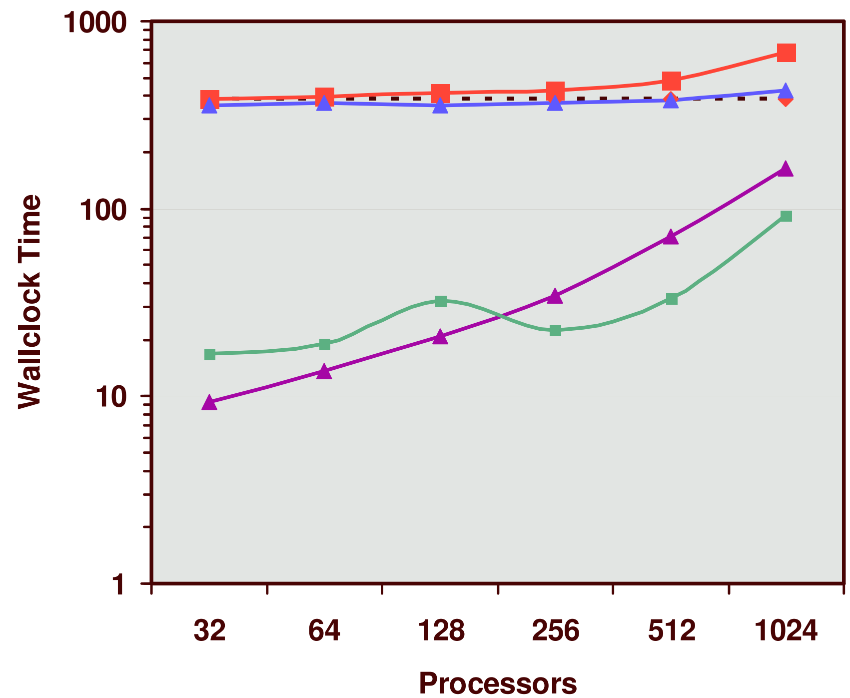


Non-scaled
4 level Euler Problem
IBM Blue Pacific



Scaled
3 level linear advection
Linux MCR Cluster





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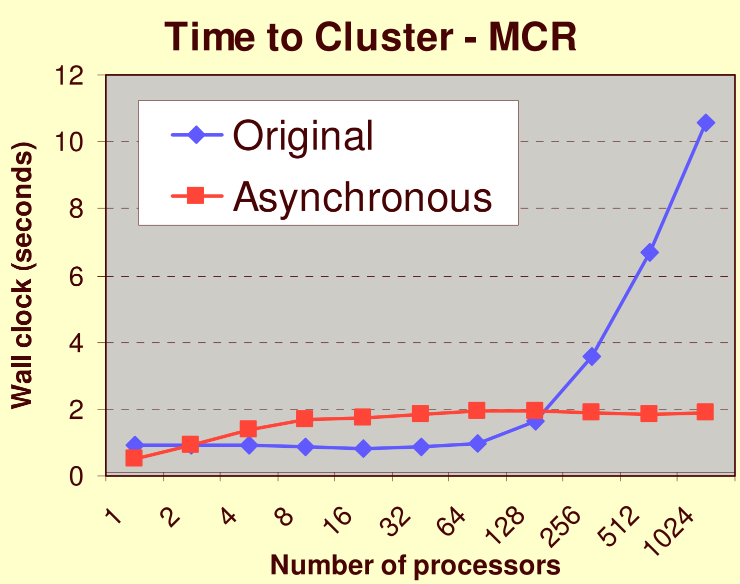
- **Predictions of scaling issues on O(100,000) processors**

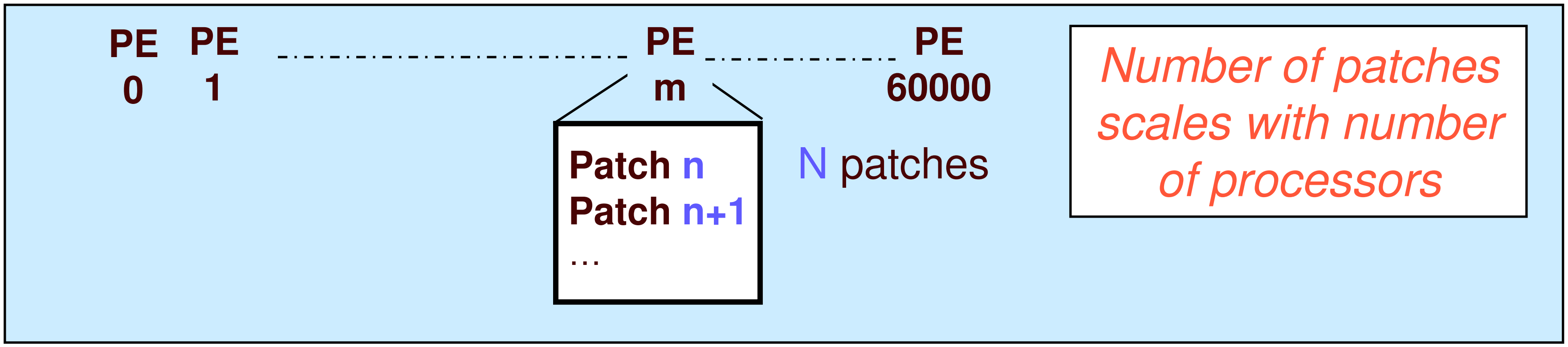
A new asynchronous clustering algorithm for very large scale parallel systems

- **Our new clustering algorithm is effective in reducing costs on O(1K) processors, but not O(10K)-O(100K) processors.**
- **Results from an asynchronous implementation will be presented (B. Gunney – Tues afternoon session CP44)**



Asynchronous implementation avoids global communication and synchronization

More efficient graph-based algorithms required for O(10K)-O(100K) procs



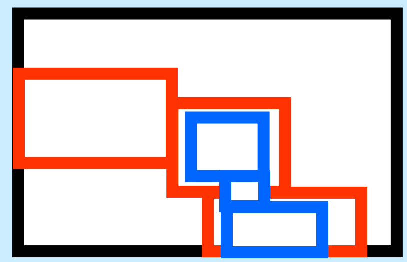
- Naive implementation of box operations in gridding may invoke O(N^2) algorithms (e.g. former communication schedule algorithm).
- We've developed more efficient graph-based algorithms that work on up to O(1000) processors, but ***further work will be required***
- Difficult to assess beforehand because complexity is generally problem dependent.

Storage of globally-known information may introduce memory issues

- **Current approach: Patch lower/upper indices (i.e. “box”) known <u>globally</u> by every MPI process (to determine data locality, communication dependencies, etc.)**

requires consistency across processors: e.g.

```
BoxList boxes = level->getBoxes();
```



- **Because # patches grows with # processors, trivial overhead may become non-trivial on very large scale parallel systems**

procs	patches	per processor storage (MB)
0.5K	2.5K-10K	< 1 MB
60K	300K-1200K	20-80MB

Large overhead for nodes of BG/L

Concluding Remarks

- **Fully adaptive calculations are scalable to O(1000) processors**
- **Adaptive gridding costs are our largest source of parallel inefficiency**
  - Communication is cheap and scales well
  - Re-gridding operations that are trivial on small numbers of processors become significant on large numbers.
  - Tree-based algorithms successful in reducing these costs.
- **Further work required to handle O(100K) processors**
  - New Berger-Rigoutsos clustering algorithm proposed
  - Continued exploration into more efficient tree-based representations of spatial relationships between patches